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Dynamical Systems on Statistical Models

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Abstract

Dualistic properties of a gradient flow on a manifold M associated with a dualistic structure (g, ∇, ∇^*) is studied from an information geometrical viewpoint. Statistical significance of the gradient flow is also investigated.

1 Introduction

Motivated mainly by classical mechanics, completely integrable dynamical systems have been investigated by many researchers. Furthermore, some authors have sought contacts with other fields such as linear programming [4] and eigenvalue problems of matrices [5], see also [6] and the references cited therein.

On the other hand, some physicists have studied nonequilibrium or dissipative processes from a geometrical viewpoint [3]. Obata et al. also examined some nonequilibrium processes by using information geometry [9]. They showed the Uhlenbeck–Ornstein process is a geodesic motion with respect to the exponential connection on a Gaussian model.

Quite recently, Nakamura pointed out that certain gradient flows on Gaussian and multinomial distributions can be characterized as completely integrable Hamiltonian systems [8]. This is the first suggestion of the connection between two seemingly unrelated fields, i.e., information geometry and completely integrable dynamical systems.

In this paper, general dualistic properties of a gradient flow on a manifold M associated with a dualistic structure (g, ∇, ∇^*) is studied from an information geometrical point of view. Statistical significance of the gradient flow is also investigated.

2 Dualistic geometry

We first give a brief summary of dualistic geometry. For details, consult [2]. Let M be a Riemannian manifold with metric g . Two affine connections ∇ and ∇^* on M are said to be *dual* with respect to g if for any vector field A , B , and C on M ,

$$Ag(B|C) = g(\nabla_A B|C) + g(B|\nabla_A^* C),$$

where $g(B|C)$ denotes the inner product of B and C with respect to the metric g . If the torsions and the Riemannian curvatures of M with respect to the connections ∇ and ∇^* vanish, M is said to be *flat*, and a pair of divergences on M are defined in the following way. We first construct mutually dual affine coordinates on M , i.e., ∇ -affine coordinate $\theta = [\theta^i]$ and ∇^* -affine coordinate $\eta = [\eta_i]$ which satisfy

$$g(\partial_i | \partial^j) = \delta_i^j, \quad (1)$$

where $\partial_i = \partial/\partial\theta^i$ and $\partial^j = \partial/\partial\eta_j$. Then there exist such potential functions $\psi(\theta)$, $\phi(\eta)$ on M satisfying

$$\theta^i = \partial_i \phi(\eta), \quad \eta_i = \partial^i \psi(\theta), \quad \psi(\theta) + \phi(\eta) - \theta \cdot \eta = 0,$$

where $\theta \cdot \eta = \theta^i \eta_i$. By using these potentials, we define the ∇ -divergence D as

$$D(p_1 \parallel p_2) = \psi(\theta_2) + \phi(\eta_1) - \theta_2 \cdot \eta_1,$$

where η_1 and θ_2 are the η and θ coordinates of points p_1 and p_2 respectively. According to the duality, the ∇^* -divergence D^* is given as

$$D^*(p_1 \parallel p_2) = D(p_2 \parallel p_1).$$

For instance, let M be a set of positive probability distributions on a set \mathcal{X} , g the Fisher metric, ∇ and ∇^* the exponential and mixture connections, respectively. Then the exponential divergence D is given by

$$D(p_1 \parallel p_2) = \int_{\mathcal{X}} p_1(x) \log \frac{p_1(x)}{p_2(x)} dx,$$

which is identical to the Kullback–Leibler divergence $K(p_1, p_2)$. Note that our manner of naming of divergences is different from Amari's one.

Next, we tackle the converse problem, i.e., let us construct a natural dualistic structure for an arbitrary manifold M on which a potential $U(\theta)$ is given, where $\theta = [\theta^i]$ is a local coordinate system of M . In the following, we restrict ourselves to a domain Θ in which the potential $U(\theta)$ is a convex function with respect to θ . We first define another coordinate system $\eta = [\eta_i]$ and the corresponding potential $V(\eta)$ by a Legendre transformation as

$$\eta_j = \partial_j U(\theta), \quad V(\eta) = \max_{\theta \in \Theta} \{\theta^i \eta_i - U(\theta)\}.$$

Then $\theta^j = \partial^j V(\eta)$ holds, and the pair (θ, η) satisfy the identity

$$U(\theta) + V(\eta) - \theta \cdot \eta = 0.$$

The metric \hat{g} on M is defined by

$$\hat{g}_{ij} = \partial_i \partial_j U(\theta).$$

This definition can be rewritten as

$$\hat{g}_{ij} = \frac{\partial \eta_j}{\partial \theta^i},$$

which readily leads to the relation

$$\hat{g}^{ij} = \frac{\partial \theta^j}{\partial \eta_i} = \partial^i \partial^j V(\eta).$$

This indicates that the coordinate systems θ and η are mutually dual with respect to \hat{g} in the sense of Eq. (1). Further let us set

$$T_{ijk} = \partial_i \partial_j \partial_k U(\theta),$$

and define the α -connection by

$$\Gamma_{ijk}^{(\alpha)} = [ij; k] - \frac{\alpha}{2} T_{ijk},$$

with $[ij; k]$ the Levi–Civita connection, then θ and η become $\alpha = +1$ and -1 affine coordinates respectively, which can be affirmed by a straightforward computation. In this

way, a dualistic structure $(\hat{g}, \nabla^{(+1)}, \nabla^{(-1)})$ on M is derived in a natural manner from the potential $U(\theta)$. The $(+1)$ -divergence is defined as follows:

$$\begin{aligned} D^{(+1)}(p_1, p_2) &= U(\theta_2) + V(\eta_1) - \theta_2 \cdot \eta_1 \\ &= U(\theta_2) - U(\theta_1) - (\theta_2 - \theta_1) \cdot \partial_\theta U(\theta_1), \end{aligned}$$

where (θ_1, η_1) and (θ_2, η_2) are the dual affine coordinates of points $p_1, p_2 \in M$, respectively. Note that the point whose η coordinates vanish corresponds to the minimum of the potential $U(\theta)$.

3 Dualistic Dynamical Systems

In this section, we examine dualistic structures of a gradient system on a flat manifold.

Theorem 3.1 *Let M be a flat manifold with respect to the dualistic structure (g, ∇, ∇^*) , $U(p)$ a potential function on M with respect to an arbitrarily prefixed point $q \in M$ defined by*

$$U(p) = D(q \parallel p),$$

where $D(q \parallel p)$ is the ∇ -divergence. Then the gradient flow [7, p. 205]

$$\dot{\theta}^i = -g^{ij} \partial_j U(\theta) \tag{2}$$

converges to the point q along the ∇^* -geodesic, where θ is the ∇ -affine coordinates of point p , and $U(\theta) = U(p(\theta))$.

Proof Since ∇ -divergence $D(q \parallel p)$ is rewritten as

$$\begin{aligned} D(q \parallel p) &= \psi(\theta(p)) + \phi(\eta(q)) - \theta(p) \cdot \eta(q) \\ &= \psi(\theta(p)) + \{-\psi(\theta(q)) + \theta(q) \cdot \eta(q)\} - \theta(p) \cdot \eta(q) \\ &= \psi(\theta(p)) - \psi(\theta(q)) + \{\theta(q) - \theta(p)\} \cdot \eta(q), \end{aligned}$$

the gradient flow can be expressed in the form

$$\dot{\theta}^i(p) = -g^{ij} \{\partial_j \psi(\theta(p)) - \eta_j(q)\}.$$

By multiplying g_{ji} to both sides and using the identity

$$g_{ji}\dot{\theta}^i = \frac{\partial \eta_j}{\partial \theta^i} \frac{d\theta^i}{dt} = \frac{d\eta_j}{dt},$$

we have

$$\dot{\eta}_j(p) = -\{\eta_j(p) - \eta_j(q)\},$$

which can readily be integrated to obtain

$$\eta_j(p(t)) = \eta_j(q) + \{\eta_j(p(0)) - \eta_j(q)\}e^{-t}.$$

This proves the proposition. ■

Example 3.1 Here we give two examples of Theorem 3.1. Let us consider a Gaussian family with mean μ and variance σ^2 :

$$p_\theta(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp \left[-\frac{(x - \mu)^2}{2\sigma^2} \right].$$

This is a typical example of exponential family since it can be represented in the form

$$\log p_\theta(x) = \theta^1 f_1(x) + \theta^2 f_2(x) - \psi(\theta)$$

where

$$\theta^1 = \frac{\mu}{\sigma^2}, \quad \theta^2 = \frac{1}{2\sigma^2}$$

are e -affine parameters and

$$f_1(x) = x, \quad f_2(x) = -x^2, \quad \psi(\theta) = \frac{\mu^2}{2\sigma^2} + \log \sqrt{2\pi}\sigma.$$

Throughout this example, g is the Fisher metric.

We first let ∇ and ∇^* be exponential and mixture connections, respectively. Further let us set q as a δ -distribution concentrated on the origin. Then the potential becomes

$$U(\theta) = D^{(e)}(q \parallel p_\theta) = K(q, p_\theta) = \psi(\theta),$$

and the corresponding gradient flow coincides with Nakamura's dynamics [8], which converges to the δ -distribution q along an m -geodesic.

Conversely, let ∇ and ∇^* be mixture and exponential connections, respectively. Further let us set q as a uniform distribution on \mathcal{X} , then $\theta^2(q)$ vanishes and $\theta^1(q)$ remains indefinite. In this case, ∇ -affine parameters are the expectation parameters $\eta_i = E_\theta[f_i(x)]$ where $E_\theta[\cdot]$ denotes expectation at p_θ , and the dynamics takes the form

$$\dot{\eta}_i = -g_{ij}\partial^j U(\eta). \quad (3)$$

Since the potential becomes

$$U(\eta) = D^{(m)}(q \parallel p_\theta) = K(p_\theta, q) = -[\text{entropy of } p_\theta] + \text{const.},$$

the dynamics is a steepest ascent flow of entropy, which converges to the uniform distribution q along an e -geodesic. Moreover, if we rescale the time logarithmically such as

$$t \dot{\eta}_i = -g_{ij}\partial^j U(\eta), \quad (4)$$

then the dynamics can be integrated easily and expressed in the e -affine parameters as

$$\theta^j(t) = \theta^j(q) + \frac{\theta^j(0) - \theta^j(q)}{t},$$

where $\theta^j(0)$ is the e -affine coordinates of the initial point. This solution can be expressed also in the (μ, σ) space as

$$\begin{aligned} \mu(t) &= \frac{\theta^1(t)}{2\theta^2(t)} = \frac{\theta^1(0) - \theta^1(q)}{2\theta^2(0)} + \frac{\theta^1(q)}{2\theta^2(0)} t, \\ \sigma^2(t) &= \frac{1}{2\theta^2(t)} = \frac{1}{2\theta^2(0)} t. \end{aligned}$$

Here we used the relation $\theta^2(q) = 0$. If we set

$$\mu_0 = \frac{\theta^1(0) - \theta^1(q)}{2\theta^2(0)}, \quad v = \frac{\theta^1(q)}{2\theta^2(0)}, \quad D = \frac{1}{4\theta^2(0)},$$

then we have

$$\mu(t) = \mu_0 + vt, \quad \sigma^2(t) = 2Dt,$$

which shows that the dynamics (4) is nothing but a Uhlenbeck-Ornstein process [9].

Next, we consider another situation. Given a manifold M and a locally convex potential $U(\theta)$, then we can induce a natural dualistic structure $(\hat{g}, \nabla^{(+1)}, \nabla^{(-1)})$ on M by the

procedure mentioned in the previous section. Let us examine a gradient flow on M of the form

$$\dot{\theta}^i = -\hat{g}^{ij}\partial_j U(\theta), \quad (5)$$

which can be reexpressed in the dual affine coordinates as

$$\dot{\eta}_i = -\eta_i. \quad (6)$$

In case $\dim M$ is even, this dynamical system can be characterized as a completely integrable Hamiltonian system [1, p. 392], which is a generalization of Nakamura's results [8], as follows.

Theorem 3.2 *If $\dim M$ is even, say $2m$, then the dynamical system (6) is a completely integrable Hamiltonian system with position $Q_k = \eta_{2k}$, momentum $P^k = -1/\eta_{2k-1}$, and Hamiltonian $\mathcal{H} = -Q_k P^k$, ($k = 1, \dots, m$). The m quantities $\mathcal{H}_k = \eta_{2k}/\eta_{2k-1}$ are mutually independent constants of motion.*

Proof By using (6), we have

$$\dot{\mathcal{H}}_k = \frac{1}{\eta_{2k-1}^2}(\dot{\eta}_{2k}\eta_{2k-1} - \eta_{2k}\dot{\eta}_{2k-1}) = 0.$$

Independency and involutiveness of $\{\mathcal{H}_k\}_{k=1}^m$ are trivial. By straightforward computation, Hamilton's equations

$$\frac{dQ}{dt} = \frac{\partial \mathcal{H}}{\partial P^k}, \quad \frac{dP}{dt} = -\frac{\partial \mathcal{H}}{\partial Q_k}$$

are reduced to

$$\dot{\eta}_{2k} = -\eta_{2k}, \quad \dot{\eta}_{2k-1} = -\eta_{2k-1},$$

which reproduce the original gradient flow (6). ■

Note that if $\dim M$ is odd, then the dynamical system (6) can be regarded as a subdynamics of a higher dimensional completely integrable Hamiltonian system by combining it with an independent odd dimensional gradient system.

4 Constrained Dynamics on a Parametric Model

In this section, we examine a dynamical system which is induced on a parametric statistical model. Let $M = \{p_\theta\}_{\theta \in \Theta}$ be a parametric model embedded in the set of probability distributions \mathcal{P} on \mathcal{X} . Theorem 3.1 indicates that the gradient flow in \mathcal{P} with respect to the potential $U(p) = K(q_n, p)$ with q_n the empirical distribution is a dynamical system whose gradient vector is m-tangent vector from the point p toward the empirical distribution q_n which in general falls out of the model M . Therefore we can construct a constrained dynamics on the model M by projecting the gradient m-tangent vector onto the tangent space $T_p(M)$ of the model with respect to the Fisher metric.

Theorem 4.1 *Such an induced dynamical system is also a gradient flow on M of the form*

$$\dot{\theta}^i = -g^{ij} \partial_j K(q_n, p_\theta), \quad (7)$$

where g is the Fisher metric on M . This flow converges to a locally maximum likelihood estimate.

Proof Let us define a bilinear form $\langle \cdot, \cdot \rangle$ on $T_p(M)$ by

$$\langle f(x), g(x) \rangle = \int_{\mathcal{X}} f(x)g(x)dx,$$

where $f(x)$ and $g(x)$ are an m-tangent vector and an e-tangent vector, respectively. Note that this value is identical to the conventional Fisher inner product in information geometry. Then the projection of the m-tangent vector from the point p toward the empirical distribution q_n onto the tangent space $T_p(M)$, expressed as $a^i \partial_i p_\theta(x)$, satisfies

$$\langle q_n(x) - p_\theta(x), \partial_j \log p_\theta(x) \rangle = \langle a^i \partial_i p_\theta(x), \partial_j \log p_\theta(x) \rangle.$$

This leads to

$$\begin{aligned} a^i &= g^{ij} \langle q_n(x) - p_\theta(x), \partial_j \log p_\theta(x) \rangle \\ &= g^{ij} \langle q_n(x), \partial_j \log p_\theta(x) \rangle \\ &= -g^{ij} \partial_j K(q_n, p_\theta). \end{aligned}$$

Hence the induced dynamical system becomes

$$\dot{p}_\theta(x) = \dot{\theta}^i \partial_i p_\theta(x) = a^i \partial_i p_\theta(x),$$

or

$$\dot{\theta}^i = a^i = -g^{ij} \partial_j K(q_n, p_\theta).$$

Every equilibrium point of this flow satisfies $a^i = 0$ for all i , which is nothing but foots of the m -geodesic perpendiculars from q_n onto the model M . ■

Lemma 4.1 *Suppose the potential $U(\theta)$ on M is given by the Kullback-Leibler divergence, i.e., $U(\theta) = K(q_n, p_\theta)$. The induced metric $\hat{g}_{ij}(\theta)$ is identical to the Fisher metric $g_{ij}(\theta)$ for every $q_n \in \mathcal{P}$ iff the model M is an exponential family.*

Proof If $\hat{g}_{ij}(\theta)$ is identical to $g_{ij}(\theta)$ for every $q_n \in \mathcal{P}$, then

$$g_{ij}(\theta) - \hat{g}_{ij}(\theta) = - \int_{\mathcal{X}} \{p_\theta(x) - q_n(x)\} \partial_i \partial_j \log p_\theta(x) dx = 0.$$

This shows that $\partial_i \partial_j \log p_\theta(x)$ does not depend on x , i.e., there exists a function $\psi(\theta)$ such that

$$\partial_i \partial_j \log p_\theta(x) = -\partial_i \partial_j \psi(\theta)$$

holds. This equation can readily be integrated to yield

$$\log p_\theta(x) = c(x) + \theta^i f_i(x) - \psi(\theta),$$

which shows that the model $\{p_\theta(x)\}$ is an exponential family. The converse statement is evident from the calculations above. ■

Theorem 4.2 *If model M is an exponential family, then the induced gradient flow (7) converges to the unique maximum likelihood estimate with respect to the empirical distribution q_n along m -geodesic. Moreover, if $\dim M$ is even, say $2m$, then the flow is a completely integrable Hamiltonian system with position $Q_k = \partial_{2k} K(q_n, p_\theta)$, momentum $P^k = -1/\partial_{2k-1} K(q_n, p_\theta)$, and Hamiltonian $\mathcal{H} = -Q_k P^k$, $k = 1, \dots, m$.*

Proof Straightforward from Theorems 3.1, 3.2, 4.1, and Lemma 4.1. ■

5 Concluding Remarks

We have constructed a gradient flows on a flat manifold M with respect to a dualistic structure (g, ∇, ∇^*) which converges to an arbitrarily prefixed point along ∇ -geodesic. If $\dim M$ is even, this flow can be also characterized as a completely integrable Hamiltonian flow.

We have also derived a constrained dynamics on a submanifold M embedded in a statistical manifold \mathcal{P} , which converges to the locally maximum likelihood estimate. If M is an exponential family, then the flow evolves along m -geodesics. In case $\dim M$ is even, the flow can also be considered as a completely integrable Hamiltonian system. However, statistical meaning of such characterization as a Hamiltonian system is not clear.

In a basic sense, a $2n$ dimensional Hamiltonian system is equivalent to a n dimensional Lagrangean system. From this analogy, we can imagine a 2nd order dynamics of the form

$$\ddot{\theta}^k + \left\{ \begin{matrix} k \\ ij \end{matrix} \right\} \dot{\theta}^i \dot{\theta}^j = -g^{kj} \partial_j U(\theta),$$

which is the equation of motion of a particle constrained on a manifold M associated with a potential $U(\theta)$. It is well known that this dynamics can be derived by the variational principle with Lagrangean

$$\mathcal{L} = \frac{1}{2} g_{ij} \dot{\theta}^i \dot{\theta}^j - U(\theta).$$

In the same way, if we consider a dynamical system of the form

$$\ddot{\theta}^k + \Gamma_{ij}^{(-1)k} \dot{\theta}^i \dot{\theta}^j = -\hat{g}^{kj} \partial_j U(\theta),$$

then we have

$$\ddot{\eta}_i = -\eta_i$$

in the dual affine coordinates, which indicates that the system is composed of n independent harmonic oscillators and can be regarded as a completely integrable Hamiltonian system. In this case, however, it is not clear whether the system can be derived by a certain variational principle.

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